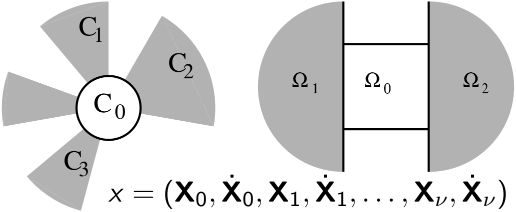
Thermostats equivalence in the thermodynamic limit for particles systems

Remembering Errico Presutti, GG

Thermostat models (Feynman-Vernon 1963): finite system in contact with infinite. Examples:



$$x = (\mathbf{X}_0, \dot{\mathbf{X}}_0, \mathbf{X}_1, \dot{\mathbf{X}}_1, \ldots, \mathbf{X}_\nu, \dot{\mathbf{X}}_\nu)$$

Initial state:

$$\mu_0(dx) \overset{def}{=} C e^{-\sum_{j=0}^{\nu} \beta_j H_j(\mathbf{X}_j, \dot{\mathbf{X}}_j)} \prod_j \frac{d\mathbf{X}_j \, d\dot{\mathbf{X}}_j}{N_j!}$$

Equations of motion:

$$
\begin{aligned}
m\ddot{\mathbf{X}}_{0i} &= -\,\partial_i U_0(\mathbf{X}_0) - \sum_{j>0} \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \partial_i \Psi(\mathbf{X}_j) + \Phi_i(\mathbf{X}_0) \\
m\ddot{\mathbf{X}}_{ji} &= -\,\partial_i U_j(\mathbf{X}_j) - \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \partial_i \Psi(\mathbf{X}_j)
\end{aligned}
$$

$$
\mathbf{U_j}(\mathbf{X_j}) = \sum_{\mathbf{q},\mathbf{q}'\in\mathbf{X_j}} \varphi(\mathbf{q}-\mathbf{q}'), \qquad \mathbf{U_{0,j}}(\mathbf{X_0}, \mathbf{X_j}) = \sum_{\mathbf{q}\in\mathbf{\Omega_0},\mathbf{q}'\in\mathbf{\Omega_j}} \varphi(\mathbf{q}-\mathbf{q}')
$$

$$
\mathbf{\Psi}(\mathbf{X}) = \sum_{\mathbf{q}\in\mathbf{X}} \psi(\mathbf{q}) \qquad\qquad (\psi(\mathbf{r}) = \mathrm{c}\,\mathbf{r}^{-\alpha}\ \ \mathbf{r} = \mathrm{distance}(\partial))
$$

Initial state: infinite Gibbs at given density δ_j and temperatures β_j^{-1}

No phase transitions $\Rightarrow$ kinetic-potential energy density, density and many observables are constant with μ_0 probability 1 at time $t = 0$: examples

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} K_{j,\Lambda}(x) = \frac{d}{2}\beta_j^{-1}\delta_j$$

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} N_{j,\Lambda}(x) = \delta_j$$

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} U_{j,\Lambda}(x) = u_j$$

Thermostats should admit evolution: defined by a limit

Regularize in a ball Λ_n (side $2^n r_\varphi$) $\Rightarrow$ Time evolution exists 4
$x \to S_t^{(n,0)} x \Rightarrow$

it should be also $\lim_{n\to\infty} S_t^{(n,0)} x = S_t^{(0)} x$ **??**

Temperature, density, energy density should be fixed $\forall t, j > 0$

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda \cap \Omega_j|} K_{j,\Lambda}(S_t^{(0)} x) = \frac{d}{2}\beta_j^{-1}\delta_j \equiv \frac{d}{2} k_B T_j \delta_j \qquad ??$$

Entropy: thermostats entropy increases by

$$\sigma_0(x) = \sum_{j>0} \frac{Q_j}{k_B T_j(x)}, \qquad Q_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_{\mathbf{X}_j} U_{0,j}(\mathbf{X}_0, \mathbf{X}_j))$$

Existence: Theorem by Caglioti, Marchioro, Pulvirenti (2000) [1]

Remarkable conclusion of a series of works by

Lanford (1968) 1 dimension (a.e. for general states) [2].

Sinai (1971) 1 dimension (a.e. for general states, proving cluster dynamics) [3].

Marchioro, Pellegrinotti, Presutti (1974) (a.e. only for Gibbs states arbitrary dim.) [4]

Dobrushin Fritz (1977) (a.e. for dim.=2 general states) [5]

$W(x;\xi,R)\overset{def}{=}$ **total energy + number of particles in ball** $\mathcal{B}(\xi,R)$

$$\mathcal{E}(x)\overset{def}{=}\sup_{\xi}\sup_{R>(\log_+(\frac{\xi}{r_\varphi}))^{1/d}}\frac{W(x;\xi,R)}{R^d}$$

Theorem: *$\exists C(\mathcal{E}), c(\mathcal{E})^{-1}$, $\uparrow\mathcal{E}$, and if $q_i(0)\in\Lambda_k$ ($v_1=\sqrt{\frac{2\varphi(0)}{m}}$)*

$$(1)\qquad |\dot q_i^{(n,0)}(t)|\le\, v_1\, C(\mathcal{E})\, k^{1/2},$$

$$(2)\qquad \mathrm{distance}\big(q_i^{(n,0)}(t),\partial(\cup_j\Omega_j\cap\Lambda_n)\big)\ge\, c(\mathcal{E})\, k^{-\frac{3}{2\alpha}}\, r_\varphi$$

$$(3)\qquad \mathcal{N}_i(t,n)\le\, C(\mathcal{E})\, k^{3/4}$$

$$(4)\qquad |x_i^{(n,0)}(t)-x_i^{(0)}(t)|\le\, C(\mathcal{E})\, r_\varphi\, e^{-c(\mathcal{E})2^{nd/2}}$$

$\forall\, n>k$. *The $x^{(0)}(t)$ is unique 0-friction motion with 1,2,3*, **[1]**

Q1: is the temperature fixed for $t > 0$? are intensive quantities constants of motion?

Q2: Alternative models (Λ_n–regularized Gaussian thermostats)

$$\begin{aligned} m\ddot{\mathbf{X}}_{0i} =& -\partial_i U_0(\mathbf{X}_0) - \sum_{j>0} \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \partial_i \Psi(\mathbf{X}_j) + \Phi_i(\mathbf{X}_0) \\ m\ddot{\mathbf{X}}_{ji} =& -\partial_i U_j(\mathbf{X}_j) - \partial_i U_{0,j}(\mathbf{X}_0, \mathbf{X}_j) + \partial_i \Psi(\mathbf{X}_j) - \alpha_{j,n}\dot{\mathbf{X}}_{ji} \end{aligned}$$

With $\alpha_{j,n}$ **so fixed that** $U_{j,\Lambda_n} + K_{j,\Lambda_n} = E_{j,\Lambda_n}$ **is exact constant**

$$\alpha_{j,n} \stackrel{def}{=} \frac{Q_j}{d\, N_j k_B T_j(x)}, \qquad Q_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$$

with $m\dot{\mathbf{X}}_j^2 \stackrel{def}{=} 2K_{j,\Lambda_n}(x) \stackrel{def}{=} d\, N_j k_B T_j(x)$

Equivalence? (in therm. lim. $\Lambda_n \to \infty$)

Idea: $Q_j \stackrel{def}{=} -\dot{\mathbf{X}}_j \cdot \partial_j U_{0,j}(\mathbf{X}_0, \mathbf{X}_j)$ **is** $O(1)$
(Williams,Searles,Evans 2004) [6]

hence $\alpha_{\mathbf{j}} = \frac{\mathbf{Q_j}}{\mathbf{d\,N_j k_B T_{j,n}(x)}} \;\Rightarrow 0$ **as** $n \to \infty$.

But is $T_{j,n}(x) \geq c > 0$ **??**

Theorem (Presutti, G): *with* μ_0*–probability* 1

(a) $\frac{\mathbf{K_{j,\Lambda_n}(x)}}{|\mathbf{\Lambda_n \cap \Omega_j}|} \;\geq \frac{1}{4}\, d\, \delta_j\, k_B\, T_j$ *(hence* $\alpha \xrightarrow[n\to\infty]{} 0$*).*

(b) $\lim_{n\to\infty} S_t^{(n,1)} x = \lim_{n\to\infty} S_t^{(n,0)} x$ **for all** $t > 0$.

(c) $\frac{d\mu_t(dx)}{dt} \;=\; -\sigma(x)\, \mu_t(dx)$ **and**

$$\sigma(\mathbf{x}) = \sum_{\mathbf{j}>\mathbf{0}} \frac{\mathbf{Q_j}}{\mathbf{k_B T_j(x)}} + \beta_{\mathbf{0}}(\dot{\mathbf{K}}_{\mathbf{0}} + \dot{\mathbf{U}}_{\mathbf{0}} + \dot{\mathbf{\Psi}}_{\mathbf{0}}) \stackrel{\mathbf{def}}{=} \sigma_{\mathbf{0}}(\mathbf{x}) + \dot{\mathbf{F}}(\mathbf{x})$$

Entropy production = volume contraction + a time derivative: $\Rightarrow$

(average of σ) $\equiv$ (average of σ_0)

provided $\beta_j(x)$ is a constant of motion as $n \to \infty$ and $\beta_j(S_t x) = \beta_j$

In other words: very generally phase space contraction can be identified with the physically defined entropy production.

i

$\Rightarrow$ **Infinitely many constants of motion: [7, 8, 9]**

Consider the averages of the following global observables:

$$\lim_{n\to\infty} \Big(\frac{N_{j,\Lambda_n}(S_t x)}{|\Lambda_n \cap \Omega_j|}, \; \frac{U_{j,\Lambda_n}(S_t x)}{|\Lambda_n \cap \Omega_j|}, \; \frac{K_{j,\Lambda_n}(S_t x)}{|\Lambda_n \cap \Omega_j|} \Big)$$

Theorem 1: *The limits exist with μ_0-probability 1 for all times and are time independent. The limits will be respectively δ_j, u_j and $\frac{d}{2}\delta_j kBT_j$ with μ_0-prob.$=1$.*

More generally if $G_\Lambda(x)=\sum_{X\subset\Lambda,(X,Y)\in x} G(X,Y)$ **suppose** $H_{0,\Lambda,G}(x)\stackrel{def}{=}H_{0,\Lambda}(x)+\varepsilon G_\Lambda(x)$ **superstable for** $|\varepsilon|$ **small**

(*i.e.* exist $a>0, b\ge 0$ and for all Λ it is, $\forall x=(X,\dot X)$ with N particles, $X\subset\Lambda$ and $|\varepsilon|$: $H_{0,\Lambda,\Gamma}(x)\ge aN^2/|\Lambda|-bN$).

Call G **an "***allowed observable***".**

For such observables define, for $|\varepsilon|$ **small, the "pressure"** $P(\varepsilon)=\lim_{\Lambda\to\infty}\frac{1}{|V|}\log\frac{Z_j(\varepsilon)}{Z_j(0)}$. **Then:**

Theorem 2: *Let G be an allowed observable. If $P(\varepsilon)$ is differentiable at $\varepsilon=0$, then with μ_0–probability 1 the limit as $n\to\infty$ of $\frac{1}{|\Lambda_n|}G_{\Lambda_n}(S_t x)$ exists μ_0–a.e. and is t-independent.*

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